

Isobutylmalonic acid
4361-06-2 | DTXSID60195885

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 6.48e-01

Global applicability domain: Inside

Local applicability domain index: 6.45e-01

Confidence level: 6.88e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2,2-Dimethylpentanedioic acid</div> <div>Measured: 0.67</div> <div>Predicted: 7.43e-01</div>	<div>Image not found</div> <div>Heptanedioic acid</div> <div>Measured: 0.61</div> <div>Predicted: 6.46e-01</div>	<div>Image not found</div> <div>4-oxo-2-propylpentanoic acid</div> <div>Measured: 1.31</div> <div>Predicted: 1.27</div>
<div>Image not found</div> <div>Propanedioic acid, dimethyl-</div> <div>Measured: 0.39</div> <div>Predicted: 2.43e-01</div>	<div>Image not found</div> <div>Hexanedioic acid</div> <div>Measured: 0.08</div> <div>Predicted: 6.25e-02</div>	